# Stopping molecular rotation using coherent ultra-low-energy magnetic manipulations.

## Content

The most detailed insights into collisions at a molecular level are provided by quantum state resolved experiments, as they remove the averaging over the many degrees of freedom that can influence the outcome of the collision. One quantum state that was particularly difficult to control for ground state molecules is the rotational orientation projection ($m_J$) state. This limitation has recently been overcome, with the development of a magnetic manipulation technique [1] which has made it possible to coherently control the $m_J$ (and nuclear spin projection, $m_I$) states of small ground state molecules. Here, the unique methodology will be presented using a recent study of the rotationally inelastic scattering of D<sub>2</sub> from a Cu(111) surface [2] as an example. In these experiments, the $m_J$ state of the incoming D<sub>2</sub> molecule in the rotational state $J$ = 2 was controlled and manipulated and was shown to change the probability that the D<sub>2</sub> molecule inelastically scattered into the $J$ = 0 rotational state, which effectively means that an energy perturbation on the order of peV changed the probability the molecule lost 22 meV of rotational energy in the collision. The results from state of the art calculations predict that only molecules in the $m_J$ = 0 state of $J$ = 2 undergo this rotationally inelastic transition when D<sub>2</sub> scatters from Cu(111), but this does not reproduce the experimental data. Therefore, these, and similar [3], measurements provide an extremely stringent benchmark for the development of accurate theoretical models, potentially for the scattering of a range of small molecules both in the gas-phase and at the gas-surface interface.

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**References**

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[2] H. Chadwick et al., "Stopping molecular rotation using coherent ultra-low energy magnetic manipulations", Nature Communications 13, 2287 (2022).

[3] Y. Alkoby et al., "Setting benchmarks for modelling gas-surface interactions using coherent control of rotational orientation states" Nature Communications 11, 3110 (2020).

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